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10a-Hydroxy-9-[2-(trifluoromethyl)phenyl]-3,4,5,6,7,8a,9,10a-octahydro-1*H*-xanthene-1,8(2*H*)-dione

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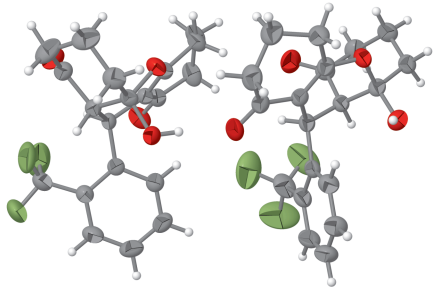
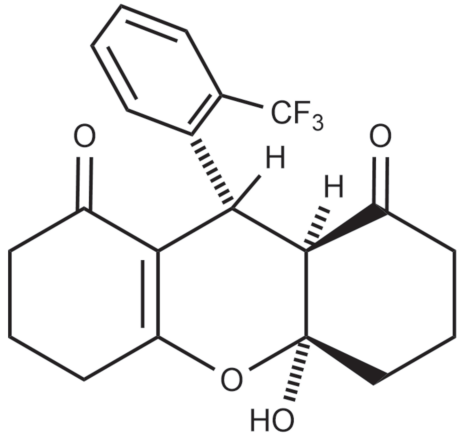
Structural data: full structural data are available from iucrdata.iucr.org

The title compound, $C_{20}H_{19}F_3O_4$, crystallizes with two independent molecules with similar geometry. In both molecules the tetrahydropyran, cyclohexene and cyclohexane rings of the xanthene moiety adopt half-chair, half-boat and chair conformations, respectively. In the extended structure, O—H···O hydrogen bonds between hydroxy and carbonyl groups link molecules into chains propagating along [100].

3D view



Chemical scheme



Structure description

Xanthene derivatives constitute a prominent class of oxygen-containing heterocycles that are gaining attention owing to their biological activities and diverse industrial applications (Ran *et al.*, 2025, Taghartapeh *et al.*, 2017, Faryabi *et al.*, 2025).

The title compound, $C_{20}H_{19}F_3O_4$, crystallizes with two independent molecules (1 and 2, shown in Figs. 1 and 2, respectively), with similar geometry. The tetrahydropyran rings adopts a half chair conformation with puckering parameters for molecules 1 and 2 of Q = 0.448 (3) Å, θ = 126.4 (4)°, φ = 87.7 (5)° and Q = 0.451 (3) Å, θ = 54.5 (4)° φ = 268.9 (4)°, respectively. The cyclohexene (C9–C14 and C29–C34) and cyclohexane (C15–C20 and C35–C40) rings adopt half-boat and chair conformations, respectively. The mean plane of the tetrahydropyran ring [r.m.s deviation = 0.183 and 0.184 Å] forms dihedral angles of 81.44 (9) and 78.75 (9) ° with the trifluoromethylphenyl ring in molecules 1 and 2, respectively. The crystal structure is further consolidated by intramolecular C20—H···F1 and C40—H···F5 interactions (Table 1).

For related structures, see Ahmed *et al.*, 2024, Fun *et al.*, 2012, Karimian *et al.*, 2025, Li 2017, Li *et al.*, 2017, Patil *et al.*, 2025, and Pesyan *et al.*, 2020).

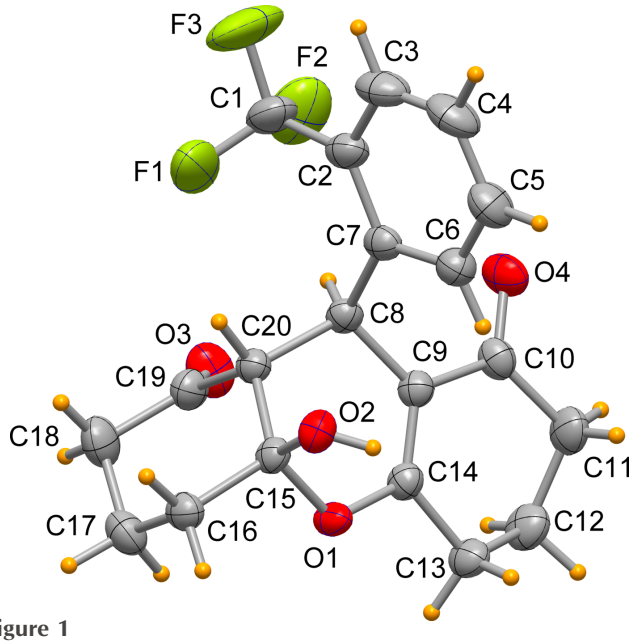


Figure 1
Displacement ellipsoid view (40% probability level) of molecule 1.

In the crystal, the molecules are linked by O2—H2···O8^{i} and O6—H6*A*···O4 hydrogen bonds (Table 1, Fig. 3), forming chains of alternating *A* and *B* molecules along [100]. Additional C—H···O interactions reinforce the structure.

Synthesis and crystallization

1,3-Cyclohexandione (2 mol), 2-(trifluoromethyl)benzaldehyde (1 mol) and nicotinic acid (10 mol %) were placed into a round-bottom flask. All the starting components were initially mixed with a glass rod. Ethanol (5 ml) was then added to the flask and the reaction mixture was heated at 60–65°C over a period of 5 h with an efficient $CaCl_2$ guard tube at the top of the condenser. After completion (TLC checked) single crystals were obtained by slow evaporation of the solvent.

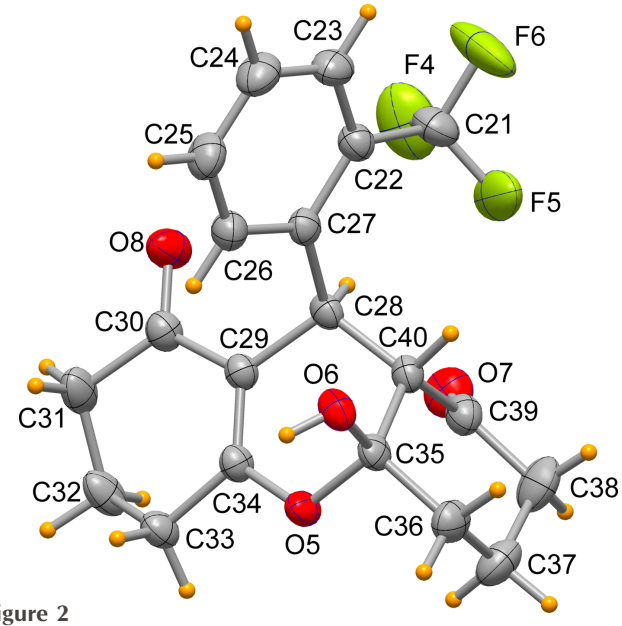


Figure 2
Displacement ellipsoid view (40% probability level) of molecule 2.

Table 1
Hydrogen-bond geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C20—H20···F1	0.98	2.40	2.960 (4)	116
C40—H40···F5	0.98	2.35	2.901 (4)	115
C11—H11*A*···F4^{i}	0.97	2.51	3.307 (5)	140
O2—H2···O8^{i}	0.89 (4)	1.82 (4)	2.704 (3)	172 (3)
O6—H6*A*···O4	0.86 (4)	1.83 (4)	2.684 (3)	171 (3)
C16—H16*B*···O2^{ii}	0.97	2.52	3.403 (4)	152
C36—H36*B*···O6^{iii}	0.97	2.59	3.473 (4)	152

Symmetry codes: (i) $x-1, y, z$; (ii) $-x, -y+2, -z+1$; (iii) $-x+1, -y+1, -z+2$.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{20}H_{19}F_3O_4$
M_r	380.35
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	293
a, *b*, *c* (Å)	10.408 (3), 11.227 (4), 15.455 (5)
α, β, γ (°)	86.17 (1), 85.465 (9), 85.919 (10)
V (Å^3)	1792.3 (10)
Z	4
Radiation type	Mo *K*α
μ (mm^{-1})	0.12
Crystal size (mm)	0.28 × 0.25 × 0.24
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.890, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	47730, 6616, 4728
R_{int}	0.064
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.605
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.068, 0.150, 1.08
No. of reflections	6616
No. of parameters	493
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.49, −0.34

Computer programs: *SMART* and *SAINT* (Bruker, 2012), *SHELXT2014/5* (Sheldrick, 2015*a*), *SHELXL2019/2* (Sheldrick, 2015*b*), *DIAMOND* (Brandenburg, 1999) and *WinGX* (Farrugia, 2012).

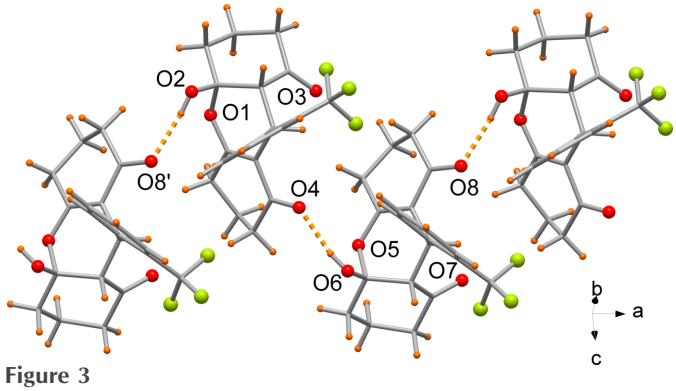


Figure 3
Crystal packing showing the molecules hydrogen-bonded along the *a*-axis direction. Symmetry code: (′) $x-1, y, z$.

The isolated yields was 90%. Color: white, m.p. 268–269°C; IR (KBr): (ν) = 2945, 2922, 2866, 1650, 1569, 1492, 1359, 1181 cm^{-1}.

^{1}H NMR (400 MHz, $CDCl_3$): δ (p.p.m.) = 12.3 (*s*, 1H, *t*-OH), 7.56–7.51 (*m*, 3H, Ar—H), 7. 45–7.39 (*m*, 1H, Ar—H), 5.72 (*s*, 1H, condensing carbon, *ali*-CH), 2.27–2.08 (*m*, 3H, *ali*-CH_2), 2.07–1.81 (*m*, 5H *ali*-CH_2), 1.80–21.72 (*m*, 5H, *ali*-CH_2);

^{13}C NMR (400 MHz, $CDCl_3$): δ (p.p.m.) = 196.0 (C═O), 151.6, 139.2, 133.2, 130.9, 129.9, 129.4, 126.2, 115.8, 136.6, 33.8, 28.6, 21.1, 19.5;

HRMS (ESI): Calculated for $C_{20}H_{19}F_3O_4$: 380.1257, found $[m/z, M + H]^+$ 381.1259.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Acknowledgements

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full crystallographic data

IUCrData (2026). **11**, x260837 [https://doi.org/10.1107/S2414314626008370]

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Crystal data

$C_{20}H_{19}F_3O_4$
M_r = 380.35
Triclinic, $P\overline{1}$
a = 10.408 (3) Å
b = 11.227 (4) Å
c = 15.455 (5) Å
α = 86.17 (1)°
β = 85.465 (9)°
γ = 85.919 (10)°
V = 1792.3 (10) Å^3
Z = 4
$F(000)$ = 792
D_x = 1.410 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9858 reflections
θ = 2.3–23.5°
μ = 0.12 mm^{-1}
T = 293 K
Block, colourless
0.28 × 0.25 × 0.24 mm

Data collection

Bruker APEX-II CCD diffractometer
φ and ω scans
Absorption correction: multi-scan SADABS-2016/2 (Bruker, 2016) was used for absorption correction.
T_{min} = 0.890, T_{max} = 1.000
47730 measured reflections
6616 independent reflections
4728 reflections with $I > 2\sigma(I)$
R_{int} = 0.064
θ_{max} = 25.5°, θ_{min} = 2.3°
h = −12→12
k = −13→13
l = −18→18

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.068
$wR(F^2)$ = 0.150
S = 1.08
6616 reflections
493 parameters
0 restraints
Primary atom site location: dual
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0398P)^2 + 2.0212P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.49 e Å^{-3}
$\Delta\rho_{min}$ = −0.34 e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.04685 (19)	0.68197 (16)	0.53497 (12)	0.0415 (5)
O2	−0.0425 (2)	0.87204 (19)	0.56390 (14)	0.0438 (5)
H2	−0.079 (3)	0.824 (3)	0.606 (2)	0.066*
O3	0.3864 (2)	0.7371 (2)	0.49268 (15)	0.0636 (7)
O4	0.3004 (2)	0.6726 (2)	0.77485 (14)	0.0550 (6)
F1	0.3711 (3)	1.0243 (3)	0.57110 (17)	0.1064 (10)
F2	0.4615 (2)	0.9443 (3)	0.6775 (2)	0.1194 (10)
F3	0.4163 (3)	1.1293 (3)	0.6713 (2)	0.1344 (13)
C1	0.3690 (4)	1.0278 (4)	0.6559 (3)	0.0674 (11)
C2	0.2420 (3)	1.0077 (3)	0.7041 (2)	0.0477 (8)
C3	0.1932 (4)	1.0930 (3)	0.7619 (2)	0.0625 (10)
H3	0.239538	1.159417	0.767991	0.075*
C4	0.0780 (4)	1.0802 (3)	0.8097 (2)	0.0666 (11)
H4	0.045018	1.138552	0.846931	0.080*
C5	0.0118 (4)	0.9805 (3)	0.8022 (2)	0.0584 (9)
H5	−0.065546	0.970241	0.835460	0.070*
C6	0.0593 (3)	0.8958 (3)	0.74568 (19)	0.0465 (8)
H6	0.013325	0.828457	0.741935	0.056*
C7	0.1736 (3)	0.9073 (2)	0.69395 (18)	0.0379 (7)
C8	0.2197 (3)	0.8123 (2)	0.62960 (17)	0.0357 (6)
H8	0.314129	0.804622	0.629212	0.043*
C9	0.1742 (3)	0.6898 (2)	0.65594 (18)	0.0360 (6)
C10	0.2229 (3)	0.6260 (3)	0.73309 (19)	0.0417 (7)
C11	0.1763 (4)	0.5050 (3)	0.7607 (2)	0.0552 (9)
H11A	0.098290	0.514546	0.798925	0.066*
H11B	0.241261	0.459728	0.793374	0.066*
C12	0.1487 (4)	0.4354 (3)	0.6851 (2)	0.0577 (9)
H12A	0.229107	0.413747	0.652041	0.069*
H12B	0.109643	0.362262	0.706691	0.069*
C13	0.0595 (3)	0.5076 (3)	0.6269 (2)	0.0473 (8)
H13A	0.059302	0.469250	0.572560	0.057*
H13B	−0.027678	0.509462	0.654392	0.057*
C14	0.0984 (3)	0.6330 (2)	0.60840 (18)	0.0372 (7)
C15	0.0550 (3)	0.8093 (2)	0.51477 (18)	0.0359 (7)
C16	0.0307 (3)	0.8283 (3)	0.41956 (18)	0.0429 (7)
H16A	−0.049301	0.793471	0.410035	0.052*
H16B	0.019897	0.913485	0.404574	0.052*
C17	0.1380 (3)	0.7741 (3)	0.3599 (2)	0.0540 (9)
H17A	0.119369	0.793308	0.299851	0.065*

H17B	0.143170	0.687774	0.369897	0.065*
C18	0.2669 (3)	0.8221 (3)	0.3760 (2)	0.0583 (9)
H18A	0.335698	0.783960	0.339382	0.070*
H18B	0.264485	0.907600	0.361675	0.070*
C19	0.2922 (3)	0.7966 (3)	0.4700 (2)	0.0451 (7)
C20	0.1882 (3)	0.8468 (2)	0.53492 (17)	0.0350 (6)
H20	0.186337	0.934216	0.526943	0.042*
O5	0.52022 (19)	0.45581 (17)	0.77075 (11)	0.0395 (5)
O6	0.4547 (2)	0.56409 (19)	0.89156 (13)	0.0429 (5)
H6A	0.401 (3)	0.592 (3)	0.855 (2)	0.064*
O7	0.8591 (2)	0.3713 (2)	0.82021 (16)	0.0597 (6)
O8	0.8265 (2)	0.7386 (2)	0.68871 (13)	0.0546 (6)
F4	0.9888 (2)	0.6603 (3)	0.90155 (18)	0.1099 (10)
F5	0.8719 (2)	0.5522 (2)	0.98249 (19)	0.0968 (9)
F6	0.9442 (3)	0.7017 (3)	1.03118 (19)	0.1174 (11)
C21	0.8932 (3)	0.6659 (3)	0.9643 (2)	0.0536 (9)
C22	0.7793 (3)	0.7418 (3)	0.93647 (18)	0.0394 (7)
C23	0.7544 (3)	0.8500 (3)	0.9753 (2)	0.0483 (8)
H23	0.806566	0.869800	1.017658	0.058*
C24	0.6539 (4)	0.9279 (3)	0.9519 (2)	0.0570 (9)
H24	0.637967	1.000232	0.978143	0.068*
C25	0.5769 (3)	0.8985 (3)	0.8894 (2)	0.0537 (9)
H25	0.508855	0.951256	0.872990	0.064*
C26	0.5999 (3)	0.7914 (3)	0.85095 (19)	0.0436 (7)
H26	0.546408	0.772878	0.808982	0.052*
C27	0.7011 (3)	0.7096 (2)	0.87305 (17)	0.0354 (6)
C28	0.7244 (3)	0.5918 (2)	0.82750 (16)	0.0336 (6)
H28	0.818334	0.575745	0.820355	0.040*
C29	0.6773 (3)	0.5996 (2)	0.73701 (17)	0.0333 (6)
C30	0.7382 (3)	0.6793 (3)	0.67074 (18)	0.0398 (7)
C31	0.6901 (3)	0.6886 (3)	0.58137 (19)	0.0535 (9)
H31A	0.758336	0.714790	0.539497	0.064*
H31B	0.618061	0.748161	0.579322	0.064*
C32	0.6475 (3)	0.5703 (3)	0.55668 (19)	0.0523 (9)
H32A	0.721407	0.512742	0.552333	0.063*
H32B	0.611718	0.580587	0.500382	0.063*
C33	0.5470 (3)	0.5239 (3)	0.62410 (17)	0.0430 (7)
H33A	0.465701	0.570467	0.617923	0.052*
H33B	0.533717	0.441438	0.614226	0.052*
C34	0.5866 (3)	0.5310 (3)	0.71430 (17)	0.0347 (6)
C35	0.5311 (3)	0.4650 (3)	0.86283 (16)	0.0356 (7)
C36	0.4825 (3)	0.3502 (3)	0.9050 (2)	0.0481 (8)
H36A	0.396614	0.340900	0.887314	0.058*
H36B	0.476211	0.354804	0.967630	0.058*
C37	0.5696 (4)	0.2417 (3)	0.8810 (2)	0.0615 (10)
H37A	0.569984	0.232216	0.819105	0.074*
H37B	0.536897	0.170581	0.911653	0.074*
C38	0.7067 (4)	0.2559 (3)	0.9048 (3)	0.0671 (11)

H38A	0.707532	0.256271	0.967515	0.081*
H38B	0.762475	0.188339	0.885607	0.081*
C39	0.7573 (3)	0.3695 (3)	0.8637 (2)	0.0451 (8)
C40	0.6712 (3)	0.4828 (2)	0.87970 (17)	0.0349 (6)
H40	0.672393	0.497469	0.941421	0.042*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0531 (13)	0.0306 (11)	0.0429 (11)	−0.0079 (9)	−0.0173 (9)	0.0036 (9)
O2	0.0420 (12)	0.0407 (12)	0.0470 (12)	−0.0020 (10)	0.0029 (10)	0.0024 (10)
O3	0.0480 (14)	0.0805 (18)	0.0593 (15)	0.0146 (13)	0.0011 (12)	−0.0070 (13)
O4	0.0642 (15)	0.0517 (14)	0.0507 (13)	0.0026 (11)	−0.0248 (12)	0.0013 (11)
F1	0.0952 (19)	0.155 (3)	0.0752 (17)	−0.0707 (18)	0.0063 (14)	−0.0001 (16)
F2	0.0553 (15)	0.141 (3)	0.159 (3)	−0.0068 (16)	−0.0117 (16)	0.022 (2)
F3	0.118 (2)	0.114 (2)	0.182 (3)	−0.080 (2)	0.019 (2)	−0.051 (2)
C1	0.064 (3)	0.066 (3)	0.077 (3)	−0.030 (2)	−0.021 (2)	0.000 (2)
C2	0.053 (2)	0.0436 (19)	0.0494 (18)	−0.0087 (15)	−0.0183 (15)	−0.0015 (15)
C3	0.083 (3)	0.042 (2)	0.068 (2)	−0.0047 (19)	−0.029 (2)	−0.0146 (18)
C4	0.089 (3)	0.060 (2)	0.054 (2)	0.010 (2)	−0.018 (2)	−0.0252 (18)
C5	0.064 (2)	0.064 (2)	0.0469 (19)	0.0040 (19)	−0.0018 (16)	−0.0138 (17)
C6	0.052 (2)	0.0456 (19)	0.0421 (17)	−0.0054 (15)	−0.0042 (15)	−0.0050 (14)
C7	0.0436 (17)	0.0342 (16)	0.0370 (15)	−0.0015 (13)	−0.0133 (13)	−0.0001 (12)
C8	0.0315 (15)	0.0374 (16)	0.0388 (15)	−0.0039 (12)	−0.0062 (12)	−0.0007 (13)
C9	0.0371 (16)	0.0326 (16)	0.0377 (15)	0.0003 (12)	−0.0033 (12)	−0.0007 (12)
C10	0.0447 (18)	0.0415 (18)	0.0380 (16)	0.0049 (14)	−0.0057 (14)	0.0000 (14)
C11	0.063 (2)	0.051 (2)	0.0500 (19)	−0.0041 (17)	−0.0123 (16)	0.0155 (16)
C12	0.067 (2)	0.0393 (19)	0.065 (2)	−0.0029 (17)	−0.0107 (18)	0.0100 (16)
C13	0.060 (2)	0.0325 (17)	0.0505 (19)	−0.0058 (15)	−0.0114 (15)	0.0023 (14)
C14	0.0384 (16)	0.0329 (16)	0.0398 (16)	−0.0018 (13)	−0.0041 (13)	0.0017 (13)
C15	0.0403 (16)	0.0286 (15)	0.0384 (15)	−0.0027 (13)	−0.0047 (13)	0.0031 (12)
C16	0.0499 (19)	0.0389 (17)	0.0407 (17)	−0.0037 (14)	−0.0111 (14)	0.0022 (13)
C17	0.069 (2)	0.055 (2)	0.0382 (17)	0.0025 (17)	−0.0087 (16)	−0.0047 (15)
C18	0.058 (2)	0.073 (2)	0.0411 (18)	−0.0002 (18)	0.0060 (16)	−0.0005 (17)
C19	0.0421 (19)	0.0486 (19)	0.0442 (18)	−0.0063 (15)	0.0018 (14)	−0.0025 (14)
C20	0.0381 (16)	0.0319 (15)	0.0353 (15)	−0.0034 (12)	−0.0060 (12)	−0.0001 (12)
O5	0.0469 (12)	0.0437 (12)	0.0294 (10)	−0.0101 (9)	−0.0047 (9)	−0.0023 (9)
O6	0.0438 (12)	0.0473 (13)	0.0371 (11)	0.0093 (10)	−0.0078 (9)	−0.0070 (9)
O7	0.0517 (15)	0.0551 (15)	0.0696 (16)	0.0111 (11)	0.0043 (13)	−0.0107 (12)
O8	0.0544 (14)	0.0683 (16)	0.0431 (12)	−0.0248 (12)	−0.0008 (10)	0.0002 (11)
F4	0.0603 (15)	0.158 (3)	0.104 (2)	0.0293 (16)	0.0009 (14)	−0.0002 (18)
F5	0.0913 (17)	0.0607 (15)	0.145 (2)	0.0035 (12)	−0.0719 (17)	0.0120 (14)
F6	0.123 (2)	0.122 (2)	0.120 (2)	0.0422 (18)	−0.0879 (18)	−0.0622 (18)
C21	0.053 (2)	0.061 (2)	0.0498 (19)	−0.0016 (17)	−0.0139 (17)	−0.0173 (17)
C22	0.0419 (17)	0.0417 (17)	0.0350 (15)	−0.0018 (14)	−0.0047 (13)	−0.0033 (13)
C23	0.062 (2)	0.0445 (19)	0.0405 (17)	−0.0080 (16)	−0.0055 (15)	−0.0099 (15)
C24	0.079 (3)	0.0370 (19)	0.054 (2)	0.0008 (18)	0.0000 (18)	−0.0100 (16)
C25	0.064 (2)	0.0389 (19)	0.056 (2)	0.0108 (16)	−0.0069 (17)	0.0004 (16)

C26	0.0496 (19)	0.0393 (18)	0.0417 (17)	0.0004 (14)	−0.0083 (14)	−0.0001 (14)
C27	0.0406 (16)	0.0364 (16)	0.0285 (14)	−0.0014 (13)	−0.0014 (12)	0.0008 (12)
C28	0.0328 (15)	0.0368 (16)	0.0314 (14)	0.0035 (12)	−0.0069 (12)	−0.0033 (12)
C29	0.0338 (15)	0.0361 (16)	0.0295 (14)	−0.0004 (12)	−0.0019 (11)	−0.0025 (12)
C30	0.0370 (17)	0.0465 (18)	0.0353 (16)	−0.0015 (14)	−0.0008 (13)	−0.0021 (13)
C31	0.053 (2)	0.071 (2)	0.0368 (17)	−0.0166 (17)	−0.0049 (15)	0.0141 (16)
C32	0.0465 (19)	0.082 (3)	0.0292 (15)	−0.0087 (17)	−0.0017 (13)	−0.0043 (16)
C33	0.0455 (18)	0.0526 (19)	0.0323 (15)	−0.0075 (15)	−0.0069 (13)	−0.0045 (14)
C34	0.0352 (15)	0.0396 (16)	0.0286 (14)	−0.0014 (13)	−0.0001 (12)	−0.0018 (12)
C35	0.0435 (17)	0.0385 (16)	0.0245 (13)	−0.0017 (13)	−0.0026 (12)	−0.0020 (12)
C36	0.057 (2)	0.0471 (19)	0.0390 (17)	−0.0092 (16)	0.0020 (15)	0.0031 (14)
C37	0.081 (3)	0.0358 (19)	0.065 (2)	−0.0085 (18)	0.0079 (19)	0.0013 (16)
C38	0.076 (3)	0.039 (2)	0.081 (3)	0.0120 (18)	0.005 (2)	0.0083 (18)
C39	0.053 (2)	0.0399 (18)	0.0426 (17)	0.0055 (15)	−0.0090 (15)	−0.0030 (14)
C40	0.0395 (16)	0.0356 (16)	0.0291 (14)	0.0040 (13)	−0.0049 (12)	−0.0017 (12)

Geometric parameters (Å, º)

O1—C14	1.360 (3)	O5—C34	1.356 (3)
O1—C15	1.449 (3)	O5—C35	1.448 (3)
O2—C15	1.397 (3)	O6—C35	1.397 (3)
O2—H2	0.89 (4)	O6—H6A	0.86 (4)
O3—C19	1.208 (4)	O7—C39	1.209 (4)
O4—C10	1.236 (4)	O8—C30	1.232 (3)
F1—C1	1.313 (4)	F4—C21	1.335 (4)
F2—C1	1.340 (5)	F5—C21	1.319 (4)
F3—C1	1.316 (4)	F6—C21	1.297 (4)
C1—C2	1.489 (5)	C21—C22	1.485 (4)
C2—C3	1.395 (5)	C22—C23	1.390 (4)
C2—C7	1.399 (4)	C22—C27	1.403 (4)
C3—C4	1.369 (5)	C23—C24	1.370 (5)
C3—H3	0.9300	C23—H23	0.9300
C4—C5	1.372 (5)	C24—C25	1.375 (5)
C4—H4	0.9300	C24—H24	0.9300
C5—C6	1.374 (4)	C25—C26	1.373 (4)
C5—H5	0.9300	C25—H25	0.9300
C6—C7	1.389 (4)	C26—C27	1.395 (4)
C6—H6	0.9300	C26—H26	0.9300
C7—C8	1.533 (4)	C27—C28	1.534 (4)
C8—C9	1.505 (4)	C28—C29	1.513 (4)
C8—C20	1.543 (4)	C28—C40	1.533 (4)
C8—H8	0.9800	C28—H28	0.9800
C9—C14	1.340 (4)	C29—C34	1.342 (4)
C9—C10	1.457 (4)	C29—C30	1.452 (4)
C10—C11	1.499 (4)	C30—C31	1.501 (4)
C11—C12	1.504 (5)	C31—C32	1.511 (5)
C11—H11A	0.9700	C31—H31A	0.9700
C11—H11B	0.9700	C31—H31B	0.9700

C12—C13	1.502 (4)	C32—C33	1.511 (4)
C12—H12A	0.9700	C32—H32A	0.9700
C12—H12B	0.9700	C32—H32B	0.9700
C13—C14	1.495 (4)	C33—C34	1.493 (4)
C13—H13A	0.9700	C33—H33A	0.9700
C13—H13B	0.9700	C33—H33B	0.9700
C15—C16	1.511 (4)	C35—C36	1.507 (4)
C15—C20	1.537 (4)	C35—C40	1.531 (4)
C16—C17	1.511 (4)	C36—C37	1.514 (5)
C16—H16A	0.9700	C36—H36A	0.9700
C16—H16B	0.9700	C36—H36B	0.9700
C17—C18	1.525 (5)	C37—C38	1.522 (5)
C17—H17A	0.9700	C37—H37A	0.9700
C17—H17B	0.9700	C37—H37B	0.9700
C18—C19	1.501 (4)	C38—C39	1.497 (5)
C18—H18A	0.9700	C38—H38A	0.9700
C18—H18B	0.9700	C38—H38B	0.9700
C19—C20	1.521 (4)	C39—C40	1.526 (4)
C20—H20	0.9800	C40—H40	0.9800

C14—O1—C15	118.1 (2)	C34—O5—C35	117.9 (2)
C15—O2—H2	111 (2)	C35—O6—H6A	113 (2)
F1—C1—F3	106.8 (3)	F6—C21—F5	106.4 (3)
F1—C1—F2	103.2 (4)	F6—C21—F4	105.5 (3)
F3—C1—F2	104.1 (3)	F5—C21—F4	102.5 (3)
F1—C1—C2	115.3 (3)	F6—C21—C22	114.6 (3)
F3—C1—C2	113.7 (4)	F5—C21—C22	114.6 (3)
F2—C1—C2	112.6 (3)	F4—C21—C22	112.1 (3)
C3—C2—C7	120.4 (3)	C23—C22—C27	120.6 (3)
C3—C2—C1	117.2 (3)	C23—C22—C21	116.4 (3)
C7—C2—C1	122.4 (3)	C27—C22—C21	123.0 (3)
C4—C3—C2	120.8 (3)	C24—C23—C22	120.7 (3)
C4—C3—H3	119.6	C24—C23—H23	119.6
C2—C3—H3	119.6	C22—C23—H23	119.6
C3—C4—C5	119.4 (3)	C23—C24—C25	119.5 (3)
C3—C4—H4	120.3	C23—C24—H24	120.2
C5—C4—H4	120.3	C25—C24—H24	120.2
C4—C5—C6	120.2 (4)	C26—C25—C24	120.3 (3)
C4—C5—H5	119.9	C26—C25—H25	119.9
C6—C5—H5	119.9	C24—C25—H25	119.9
C5—C6—C7	122.2 (3)	C25—C26—C27	121.9 (3)
C5—C6—H6	118.9	C25—C26—H26	119.0
C7—C6—H6	118.9	C27—C26—H26	119.0
C6—C7—C2	116.9 (3)	C26—C27—C22	116.9 (3)
C6—C7—C8	120.1 (3)	C26—C27—C28	120.2 (2)
C2—C7—C8	123.0 (3)	C22—C27—C28	122.9 (2)
C9—C8—C7	114.0 (2)	C29—C28—C40	109.5 (2)
C9—C8—C20	109.2 (2)	C29—C28—C27	113.3 (2)

C7—C8—C20	114.2 (2)	C40—C28—C27	114.6 (2)
C9—C8—H8	106.3	C29—C28—H28	106.3
C7—C8—H8	106.3	C40—C28—H28	106.3
C20—C8—H8	106.3	C27—C28—H28	106.3
C14—C9—C10	118.2 (3)	C34—C29—C30	118.6 (2)
C14—C9—C8	123.1 (3)	C34—C29—C28	122.7 (2)
C10—C9—C8	118.5 (2)	C30—C29—C28	118.6 (2)
O4—C10—C9	119.8 (3)	O8—C30—C29	120.0 (3)
O4—C10—C11	121.3 (3)	O8—C30—C31	121.4 (3)
C9—C10—C11	118.9 (3)	C29—C30—C31	118.7 (3)
C10—C11—C12	112.9 (3)	C30—C31—C32	111.7 (3)
C10—C11—H11A	109.0	C30—C31—H31A	109.3
C12—C11—H11A	109.0	C32—C31—H31A	109.3
C10—C11—H11B	109.0	C30—C31—H31B	109.3
C12—C11—H11B	109.0	C32—C31—H31B	109.3
H11A—C11—H11B	107.8	H31A—C31—H31B	107.9
C13—C12—C11	111.0 (3)	C31—C32—C33	110.2 (3)
C13—C12—H12A	109.4	C31—C32—H32A	109.6
C11—C12—H12A	109.4	C33—C32—H32A	109.6
C13—C12—H12B	109.4	C31—C32—H32B	109.6
C11—C12—H12B	109.4	C33—C32—H32B	109.6
H12A—C12—H12B	108.0	H32A—C32—H32B	108.1
C14—C13—C12	112.1 (3)	C34—C33—C32	111.7 (2)
C14—C13—H13A	109.2	C34—C33—H33A	109.3
C12—C13—H13A	109.2	C32—C33—H33A	109.3
C14—C13—H13B	109.2	C34—C33—H33B	109.3
C12—C13—H13B	109.2	C32—C33—H33B	109.3
H13A—C13—H13B	107.9	H33A—C33—H33B	107.9
C9—C14—O1	124.2 (3)	C29—C34—O5	124.1 (2)
C9—C14—C13	125.6 (3)	C29—C34—C33	125.3 (3)
O1—C14—C13	110.2 (2)	O5—C34—C33	110.7 (2)
O2—C15—O1	109.4 (2)	O6—C35—O5	109.8 (2)
O2—C15—C16	109.2 (2)	O6—C35—C36	111.1 (2)
O1—C15—C16	105.1 (2)	O5—C35—C36	104.7 (2)
O2—C15—C20	110.2 (2)	O6—C35—C40	107.9 (2)
O1—C15—C20	109.8 (2)	O5—C35—C40	109.9 (2)
C16—C15—C20	113.1 (2)	C36—C35—C40	113.4 (2)
C17—C16—C15	113.4 (2)	C35—C36—C37	112.5 (3)
C17—C16—H16A	108.9	C35—C36—H36A	109.1
C15—C16—H16A	108.9	C37—C36—H36A	109.1
C17—C16—H16B	108.9	C35—C36—H36B	109.1
C15—C16—H16B	108.9	C37—C36—H36B	109.1
H16A—C16—H16B	107.7	H36A—C36—H36B	107.8
C16—C17—C18	110.5 (3)	C36—C37—C38	110.3 (3)
C16—C17—H17A	109.5	C36—C37—H37A	109.6
C18—C17—H17A	109.5	C38—C37—H37A	109.6
C16—C17—H17B	109.5	C36—C37—H37B	109.6
C18—C17—H17B	109.5	C38—C37—H37B	109.6

H17A—C17—H17B	108.1	H37A—C37—H37B	108.1
C19—C18—C17	109.2 (3)	C39—C38—C37	111.2 (3)
C19—C18—H18A	109.8	C39—C38—H38A	109.4
C17—C18—H18A	109.8	C37—C38—H38A	109.4
C19—C18—H18B	109.8	C39—C38—H38B	109.4
C17—C18—H18B	109.8	C37—C38—H38B	109.4
H18A—C18—H18B	108.3	H38A—C38—H38B	108.0
O3—C19—C18	122.5 (3)	O7—C39—C38	122.3 (3)
O3—C19—C20	122.2 (3)	O7—C39—C40	122.2 (3)
C18—C19—C20	115.3 (3)	C38—C39—C40	115.4 (3)
C19—C20—C15	110.1 (2)	C39—C40—C35	110.9 (2)
C19—C20—C8	111.7 (2)	C39—C40—C28	111.4 (2)
C15—C20—C8	112.8 (2)	C35—C40—C28	112.7 (2)
C19—C20—H20	107.3	C39—C40—H40	107.2
C15—C20—H20	107.3	C35—C40—H40	107.2
C8—C20—H20	107.3	C28—C40—H40	107.2

F1—C1—C2—C3	−127.2 (4)	F6—C21—C22—C23	10.0 (5)
F3—C1—C2—C3	−3.5 (5)	F5—C21—C22—C23	133.4 (3)
F2—C1—C2—C3	114.6 (4)	F4—C21—C22—C23	−110.3 (3)
F1—C1—C2—C7	53.7 (5)	F6—C21—C22—C27	−171.5 (3)
F3—C1—C2—C7	177.5 (3)	F5—C21—C22—C27	−48.1 (4)
F2—C1—C2—C7	−64.4 (4)	F4—C21—C22—C27	68.2 (4)
C7—C2—C3—C4	0.1 (5)	C27—C22—C23—C24	−0.6 (5)
C1—C2—C3—C4	−179.0 (3)	C21—C22—C23—C24	177.9 (3)
C2—C3—C4—C5	1.7 (5)	C22—C23—C24—C25	0.1 (5)
C3—C4—C5—C6	−1.5 (5)	C23—C24—C25—C26	0.4 (5)
C4—C5—C6—C7	−0.6 (5)	C24—C25—C26—C27	−0.3 (5)
C5—C6—C7—C2	2.4 (4)	C25—C26—C27—C22	−0.2 (4)
C5—C6—C7—C8	−177.8 (3)	C25—C26—C27—C28	−179.1 (3)
C3—C2—C7—C6	−2.1 (4)	C23—C22—C27—C26	0.7 (4)
C1—C2—C7—C6	176.9 (3)	C21—C22—C27—C26	−177.8 (3)
C3—C2—C7—C8	178.1 (3)	C23—C22—C27—C28	179.5 (3)
C1—C2—C7—C8	−2.9 (5)	C21—C22—C27—C28	1.1 (4)
C6—C7—C8—C9	−27.4 (4)	C26—C27—C28—C29	26.8 (4)
C2—C7—C8—C9	152.4 (3)	C22—C27—C28—C29	−152.0 (3)
C6—C7—C8—C20	99.1 (3)	C26—C27—C28—C40	−99.8 (3)
C2—C7—C8—C20	−81.1 (3)	C22—C27—C28—C40	81.3 (3)
C7—C8—C9—C14	118.2 (3)	C40—C28—C29—C34	9.8 (4)
C20—C8—C9—C14	−10.9 (4)	C27—C28—C29—C34	−119.5 (3)
C7—C8—C9—C10	−66.8 (3)	C40—C28—C29—C30	−166.5 (2)
C20—C8—C9—C10	164.1 (2)	C27—C28—C29—C30	64.2 (3)
C14—C9—C10—O4	174.8 (3)	C34—C29—C30—O8	−176.2 (3)
C8—C9—C10—O4	−0.4 (4)	C28—C29—C30—O8	0.2 (4)
C14—C9—C10—C11	−5.8 (4)	C34—C29—C30—C31	4.6 (4)
C8—C9—C10—C11	179.0 (3)	C28—C29—C30—C31	−179.0 (3)
O4—C10—C11—C12	−147.7 (3)	O8—C30—C31—C32	146.2 (3)
C9—C10—C11—C12	32.9 (4)	C29—C30—C31—C32	−34.6 (4)

C10—C11—C12—C13	−52.5 (4)	C30—C31—C32—C33	55.5 (4)
C11—C12—C13—C14	45.6 (4)	C31—C32—C33—C34	−47.2 (4)
C10—C9—C14—O1	−179.8 (3)	C30—C29—C34—O5	−177.9 (2)
C8—C9—C14—O1	−4.8 (4)	C28—C29—C34—O5	5.8 (4)
C10—C9—C14—C13	−0.7 (4)	C30—C29—C34—C33	3.8 (4)
C8—C9—C14—C13	174.4 (3)	C28—C29—C34—C33	−172.5 (3)
C15—O1—C14—C9	−11.2 (4)	C35—O5—C34—C29	11.3 (4)
C15—O1—C14—C13	169.5 (2)	C35—O5—C34—C33	−170.3 (2)
C12—C13—C14—C9	−20.2 (4)	C32—C33—C34—C29	18.5 (4)
C12—C13—C14—O1	159.1 (3)	C32—C33—C34—O5	−159.9 (3)
C14—O1—C15—O2	−80.5 (3)	C34—O5—C35—O6	77.2 (3)
C14—O1—C15—C16	162.4 (2)	C34—O5—C35—C36	−163.4 (2)
C14—O1—C15—C20	40.5 (3)	C34—O5—C35—C40	−41.4 (3)
O2—C15—C16—C17	174.2 (2)	O6—C35—C36—C37	−175.2 (3)
O1—C15—C16—C17	−68.5 (3)	O5—C35—C36—C37	66.4 (3)
C20—C15—C16—C17	51.2 (3)	C40—C35—C36—C37	−53.5 (3)
C15—C16—C17—C18	−55.8 (4)	C35—C36—C37—C38	56.6 (4)
C16—C17—C18—C19	56.8 (4)	C36—C37—C38—C39	−55.3 (4)
C17—C18—C19—O3	120.7 (4)	C37—C38—C39—O7	−127.0 (3)
C17—C18—C19—C20	−56.9 (4)	C37—C38—C39—C40	52.5 (4)
O3—C19—C20—C15	−126.0 (3)	O7—C39—C40—C35	131.7 (3)
C18—C19—C20—C15	51.6 (3)	C38—C39—C40—C35	−47.7 (3)
O3—C19—C20—C8	0.2 (4)	O7—C39—C40—C28	5.3 (4)
C18—C19—C20—C8	177.8 (3)	C38—C39—C40—C28	−174.2 (3)
O2—C15—C20—C19	−169.5 (2)	O6—C35—C40—C39	170.8 (2)
O1—C15—C20—C19	70.0 (3)	O5—C35—C40—C39	−69.5 (3)
C16—C15—C20—C19	−47.0 (3)	C36—C35—C40—C39	47.3 (3)
O2—C15—C20—C8	65.0 (3)	O6—C35—C40—C28	−63.5 (3)
O1—C15—C20—C8	−55.6 (3)	O5—C35—C40—C28	56.2 (3)
C16—C15—C20—C8	−172.6 (2)	C36—C35—C40—C28	173.0 (2)
C9—C8—C20—C19	−84.5 (3)	C29—C28—C40—C39	85.6 (3)
C7—C8—C20—C19	146.6 (2)	C27—C28—C40—C39	−145.8 (2)
C9—C8—C20—C15	40.2 (3)	C29—C28—C40—C35	−39.8 (3)
C7—C8—C20—C15	−88.7 (3)	C27—C28—C40—C35	88.8 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2···O8^{i}	0.89 (4)	1.82 (4)	2.704 (3)	172 (3)
C11—H11*A*···F4^{i}	0.97	2.51	3.307 (5)	140
C16—H16*B*···O2^{ii}	0.97	2.52	3.403 (4)	152
C20—H20···F1	0.98	2.40	2.960 (4)	116
O6—H6*A*···O4	0.86 (4)	1.83 (4)	2.684 (3)	171 (3)
C36—H36*B*···O6^{iii}	0.97	2.59	3.473 (4)	152
C40—H40···F5	0.98	2.35	2.901 (4)	115

Symmetry codes: (i) *x*−1, *y*, *z*; (ii) −*x*, −*y*+2, −*z*+1; (iii) −*x*+1, −*y*+1, −*z*+2.

full crystallographic data

IUCrData (2026). **11**, x260837 [https://doi.org/10.1107/S2414314626008370]

10a-Hydroxy-9-[2-(trifluoromethyl)phenyl]-3,4,5,6,7,8a,9,10a-octahydro-1*H*-xanthene-1,8(2*H*)-dione

Md. Mominuddin, Harendra N. Roy, Ennio Zangrando, Injamamul Hasan and Pran Gopal Karmaker

10a-Hydroxy-9-[2-(trifluoromethyl)phenyl]-3,4,5,6,7,8a,9,10a-octahydro-1*H*-xanthene-1,8(2*H*)-dione

Crystal data

$C_{20}H_{19}F_3O_4$
M_r = 380.35
Triclinic, $P\overline{1}$
a = 10.408 (3) Å
b = 11.227 (4) Å
c = 15.455 (5) Å
α = 86.17 (1)°
β = 85.465 (9)°
γ = 85.919 (10)°
V = 1792.3 (10) Å^3
Z = 4
$F(000)$ = 792
D_x = 1.410 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9858 reflections
θ = 2.3–23.5°
μ = 0.12 mm^{-1}
T = 293 K
Block, colourless
0.28 × 0.25 × 0.24 mm

Data collection

Bruker APEX-II CCD diffractometer
φ and ω scans
Absorption correction: multi-scan SADABS-2016/2 (Bruker, 2016) was used for absorption correction.
T_{min} = 0.890, T_{max} = 1.000
47730 measured reflections
6616 independent reflections
4728 reflections with $I > 2\sigma(I)$
R_{int} = 0.064
θ_{max} = 25.5°, θ_{min} = 2.3°
h = −12→12
k = −13→13
l = −18→18

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.068
$wR(F^2)$ = 0.150
S = 1.08
6616 reflections
493 parameters
0 restraints
Primary atom site location: dual
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0398P)^2 + 2.0212P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.49 e Å^{-3}
$\Delta\rho_{min}$ = −0.34 e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.04685 (19)	0.68197 (16)	0.53497 (12)	0.0415 (5)
O2	−0.0425 (2)	0.87204 (19)	0.56390 (14)	0.0438 (5)
H2	−0.079 (3)	0.824 (3)	0.606 (2)	0.066*
O3	0.3864 (2)	0.7371 (2)	0.49268 (15)	0.0636 (7)
O4	0.3004 (2)	0.6726 (2)	0.77485 (14)	0.0550 (6)
F1	0.3711 (3)	1.0243 (3)	0.57110 (17)	0.1064 (10)
F2	0.4615 (2)	0.9443 (3)	0.6775 (2)	0.1194 (10)
F3	0.4163 (3)	1.1293 (3)	0.6713 (2)	0.1344 (13)
C1	0.3690 (4)	1.0278 (4)	0.6559 (3)	0.0674 (11)
C2	0.2420 (3)	1.0077 (3)	0.7041 (2)	0.0477 (8)
C3	0.1932 (4)	1.0930 (3)	0.7619 (2)	0.0625 (10)
H3	0.239538	1.159417	0.767991	0.075*
C4	0.0780 (4)	1.0802 (3)	0.8097 (2)	0.0666 (11)
H4	0.045018	1.138552	0.846931	0.080*
C5	0.0118 (4)	0.9805 (3)	0.8022 (2)	0.0584 (9)
H5	−0.065546	0.970241	0.835460	0.070*
C6	0.0593 (3)	0.8958 (3)	0.74568 (19)	0.0465 (8)
H6	0.013325	0.828457	0.741935	0.056*
C7	0.1736 (3)	0.9073 (2)	0.69395 (18)	0.0379 (7)
C8	0.2197 (3)	0.8123 (2)	0.62960 (17)	0.0357 (6)
H8	0.314129	0.804622	0.629212	0.043*
C9	0.1742 (3)	0.6898 (2)	0.65594 (18)	0.0360 (6)
C10	0.2229 (3)	0.6260 (3)	0.73309 (19)	0.0417 (7)
C11	0.1763 (4)	0.5050 (3)	0.7607 (2)	0.0552 (9)
H11A	0.098290	0.514546	0.798925	0.066*
H11B	0.241261	0.459728	0.793374	0.066*
C12	0.1487 (4)	0.4354 (3)	0.6851 (2)	0.0577 (9)
H12A	0.229107	0.413747	0.652041	0.069*
H12B	0.109643	0.362262	0.706691	0.069*
C13	0.0595 (3)	0.5076 (3)	0.6269 (2)	0.0473 (8)
H13A	0.059302	0.469250	0.572560	0.057*
H13B	−0.027678	0.509462	0.654392	0.057*
C14	0.0984 (3)	0.6330 (2)	0.60840 (18)	0.0372 (7)
C15	0.0550 (3)	0.8093 (2)	0.51477 (18)	0.0359 (7)
C16	0.0307 (3)	0.8283 (3)	0.41956 (18)	0.0429 (7)
H16A	−0.049301	0.793471	0.410035	0.052*
H16B	0.019897	0.913485	0.404574	0.052*
C17	0.1380 (3)	0.7741 (3)	0.3599 (2)	0.0540 (9)
H17A	0.119369	0.793308	0.299851	0.065*

H17B	0.143170	0.687774	0.369897	0.065*
C18	0.2669 (3)	0.8221 (3)	0.3760 (2)	0.0583 (9)
H18A	0.335698	0.783960	0.339382	0.070*
H18B	0.264485	0.907600	0.361675	0.070*
C19	0.2922 (3)	0.7966 (3)	0.4700 (2)	0.0451 (7)
C20	0.1882 (3)	0.8468 (2)	0.53492 (17)	0.0350 (6)
H20	0.186337	0.934216	0.526943	0.042*
O5	0.52022 (19)	0.45581 (17)	0.77075 (11)	0.0395 (5)
O6	0.4547 (2)	0.56409 (19)	0.89156 (13)	0.0429 (5)
H6A	0.401 (3)	0.592 (3)	0.855 (2)	0.064*
O7	0.8591 (2)	0.3713 (2)	0.82021 (16)	0.0597 (6)
O8	0.8265 (2)	0.7386 (2)	0.68871 (13)	0.0546 (6)
F4	0.9888 (2)	0.6603 (3)	0.90155 (18)	0.1099 (10)
F5	0.8719 (2)	0.5522 (2)	0.98249 (19)	0.0968 (9)
F6	0.9442 (3)	0.7017 (3)	1.03118 (19)	0.1174 (11)
C21	0.8932 (3)	0.6659 (3)	0.9643 (2)	0.0536 (9)
C22	0.7793 (3)	0.7418 (3)	0.93647 (18)	0.0394 (7)
C23	0.7544 (3)	0.8500 (3)	0.9753 (2)	0.0483 (8)
H23	0.806566	0.869800	1.017658	0.058*
C24	0.6539 (4)	0.9279 (3)	0.9519 (2)	0.0570 (9)
H24	0.637967	1.000232	0.978143	0.068*
C25	0.5769 (3)	0.8985 (3)	0.8894 (2)	0.0537 (9)
H25	0.508855	0.951256	0.872990	0.064*
C26	0.5999 (3)	0.7914 (3)	0.85095 (19)	0.0436 (7)
H26	0.546408	0.772878	0.808982	0.052*
C27	0.7011 (3)	0.7096 (2)	0.87305 (17)	0.0354 (6)
C28	0.7244 (3)	0.5918 (2)	0.82750 (16)	0.0336 (6)
H28	0.818334	0.575745	0.820355	0.040*
C29	0.6773 (3)	0.5996 (2)	0.73701 (17)	0.0333 (6)
C30	0.7382 (3)	0.6793 (3)	0.67074 (18)	0.0398 (7)
C31	0.6901 (3)	0.6886 (3)	0.58137 (19)	0.0535 (9)
H31A	0.758336	0.714790	0.539497	0.064*
H31B	0.618061	0.748161	0.579322	0.064*
C32	0.6475 (3)	0.5703 (3)	0.55668 (19)	0.0523 (9)
H32A	0.721407	0.512742	0.552333	0.063*
H32B	0.611718	0.580587	0.500382	0.063*
C33	0.5470 (3)	0.5239 (3)	0.62410 (17)	0.0430 (7)
H33A	0.465701	0.570467	0.617923	0.052*
H33B	0.533717	0.441438	0.614226	0.052*
C34	0.5866 (3)	0.5310 (3)	0.71430 (17)	0.0347 (6)
C35	0.5311 (3)	0.4650 (3)	0.86283 (16)	0.0356 (7)
C36	0.4825 (3)	0.3502 (3)	0.9050 (2)	0.0481 (8)
H36A	0.396614	0.340900	0.887314	0.058*
H36B	0.476211	0.354804	0.967630	0.058*
C37	0.5696 (4)	0.2417 (3)	0.8810 (2)	0.0615 (10)
H37A	0.569984	0.232216	0.819105	0.074*
H37B	0.536897	0.170581	0.911653	0.074*
C38	0.7067 (4)	0.2559 (3)	0.9048 (3)	0.0671 (11)

H38A	0.707532	0.256271	0.967515	0.081*
H38B	0.762475	0.188339	0.885607	0.081*
C39	0.7573 (3)	0.3695 (3)	0.8637 (2)	0.0451 (8)
C40	0.6712 (3)	0.4828 (2)	0.87970 (17)	0.0349 (6)
H40	0.672393	0.497469	0.941421	0.042*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0531 (13)	0.0306 (11)	0.0429 (11)	−0.0079 (9)	−0.0173 (9)	0.0036 (9)
O2	0.0420 (12)	0.0407 (12)	0.0470 (12)	−0.0020 (10)	0.0029 (10)	0.0024 (10)
O3	0.0480 (14)	0.0805 (18)	0.0593 (15)	0.0146 (13)	0.0011 (12)	−0.0070 (13)
O4	0.0642 (15)	0.0517 (14)	0.0507 (13)	0.0026 (11)	−0.0248 (12)	0.0013 (11)
F1	0.0952 (19)	0.155 (3)	0.0752 (17)	−0.0707 (18)	0.0063 (14)	−0.0001 (16)
F2	0.0553 (15)	0.141 (3)	0.159 (3)	−0.0068 (16)	−0.0117 (16)	0.022 (2)
F3	0.118 (2)	0.114 (2)	0.182 (3)	−0.080 (2)	0.019 (2)	−0.051 (2)
C1	0.064 (3)	0.066 (3)	0.077 (3)	−0.030 (2)	−0.021 (2)	0.000 (2)
C2	0.053 (2)	0.0436 (19)	0.0494 (18)	−0.0087 (15)	−0.0183 (15)	−0.0015 (15)
C3	0.083 (3)	0.042 (2)	0.068 (2)	−0.0047 (19)	−0.029 (2)	−0.0146 (18)
C4	0.089 (3)	0.060 (2)	0.054 (2)	0.010 (2)	−0.018 (2)	−0.0252 (18)
C5	0.064 (2)	0.064 (2)	0.0469 (19)	0.0040 (19)	−0.0018 (16)	−0.0138 (17)
C6	0.052 (2)	0.0456 (19)	0.0421 (17)	−0.0054 (15)	−0.0042 (15)	−0.0050 (14)
C7	0.0436 (17)	0.0342 (16)	0.0370 (15)	−0.0015 (13)	−0.0133 (13)	−0.0001 (12)
C8	0.0315 (15)	0.0374 (16)	0.0388 (15)	−0.0039 (12)	−0.0062 (12)	−0.0007 (13)
C9	0.0371 (16)	0.0326 (16)	0.0377 (15)	0.0003 (12)	−0.0033 (12)	−0.0007 (12)
C10	0.0447 (18)	0.0415 (18)	0.0380 (16)	0.0049 (14)	−0.0057 (14)	0.0000 (14)
C11	0.063 (2)	0.051 (2)	0.0500 (19)	−0.0041 (17)	−0.0123 (16)	0.0155 (16)
C12	0.067 (2)	0.0393 (19)	0.065 (2)	−0.0029 (17)	−0.0107 (18)	0.0100 (16)
C13	0.060 (2)	0.0325 (17)	0.0505 (19)	−0.0058 (15)	−0.0114 (15)	0.0023 (14)
C14	0.0384 (16)	0.0329 (16)	0.0398 (16)	−0.0018 (13)	−0.0041 (13)	0.0017 (13)
C15	0.0403 (16)	0.0286 (15)	0.0384 (15)	−0.0027 (13)	−0.0047 (13)	0.0031 (12)
C16	0.0499 (19)	0.0389 (17)	0.0407 (17)	−0.0037 (14)	−0.0111 (14)	0.0022 (13)
C17	0.069 (2)	0.055 (2)	0.0382 (17)	0.0025 (17)	−0.0087 (16)	−0.0047 (15)
C18	0.058 (2)	0.073 (2)	0.0411 (18)	−0.0002 (18)	0.0060 (16)	−0.0005 (17)
C19	0.0421 (19)	0.0486 (19)	0.0442 (18)	−0.0063 (15)	0.0018 (14)	−0.0025 (14)
C20	0.0381 (16)	0.0319 (15)	0.0353 (15)	−0.0034 (12)	−0.0060 (12)	−0.0001 (12)
O5	0.0469 (12)	0.0437 (12)	0.0294 (10)	−0.0101 (9)	−0.0047 (9)	−0.0023 (9)
O6	0.0438 (12)	0.0473 (13)	0.0371 (11)	0.0093 (10)	−0.0078 (9)	−0.0070 (9)
O7	0.0517 (15)	0.0551 (15)	0.0696 (16)	0.0111 (11)	0.0043 (13)	−0.0107 (12)
O8	0.0544 (14)	0.0683 (16)	0.0431 (12)	−0.0248 (12)	−0.0008 (10)	0.0002 (11)
F4	0.0603 (15)	0.158 (3)	0.104 (2)	0.0293 (16)	0.0009 (14)	−0.0002 (18)
F5	0.0913 (17)	0.0607 (15)	0.145 (2)	0.0035 (12)	−0.0719 (17)	0.0120 (14)
F6	0.123 (2)	0.122 (2)	0.120 (2)	0.0422 (18)	−0.0879 (18)	−0.0622 (18)
C21	0.053 (2)	0.061 (2)	0.0498 (19)	−0.0016 (17)	−0.0139 (17)	−0.0173 (17)
C22	0.0419 (17)	0.0417 (17)	0.0350 (15)	−0.0018 (14)	−0.0047 (13)	−0.0033 (13)
C23	0.062 (2)	0.0445 (19)	0.0405 (17)	−0.0080 (16)	−0.0055 (15)	−0.0099 (15)
C24	0.079 (3)	0.0370 (19)	0.054 (2)	0.0008 (18)	0.0000 (18)	−0.0100 (16)
C25	0.064 (2)	0.0389 (19)	0.056 (2)	0.0108 (16)	−0.0069 (17)	0.0004 (16)

C26	0.0496 (19)	0.0393 (18)	0.0417 (17)	0.0004 (14)	−0.0083 (14)	−0.0001 (14)
C27	0.0406 (16)	0.0364 (16)	0.0285 (14)	−0.0014 (13)	−0.0014 (12)	0.0008 (12)
C28	0.0328 (15)	0.0368 (16)	0.0314 (14)	0.0035 (12)	−0.0069 (12)	−0.0033 (12)
C29	0.0338 (15)	0.0361 (16)	0.0295 (14)	−0.0004 (12)	−0.0019 (11)	−0.0025 (12)
C30	0.0370 (17)	0.0465 (18)	0.0353 (16)	−0.0015 (14)	−0.0008 (13)	−0.0021 (13)
C31	0.053 (2)	0.071 (2)	0.0368 (17)	−0.0166 (17)	−0.0049 (15)	0.0141 (16)
C32	0.0465 (19)	0.082 (3)	0.0292 (15)	−0.0087 (17)	−0.0017 (13)	−0.0043 (16)
C33	0.0455 (18)	0.0526 (19)	0.0323 (15)	−0.0075 (15)	−0.0069 (13)	−0.0045 (14)
C34	0.0352 (15)	0.0396 (16)	0.0286 (14)	−0.0014 (13)	−0.0001 (12)	−0.0018 (12)
C35	0.0435 (17)	0.0385 (16)	0.0245 (13)	−0.0017 (13)	−0.0026 (12)	−0.0020 (12)
C36	0.057 (2)	0.0471 (19)	0.0390 (17)	−0.0092 (16)	0.0020 (15)	0.0031 (14)
C37	0.081 (3)	0.0358 (19)	0.065 (2)	−0.0085 (18)	0.0079 (19)	0.0013 (16)
C38	0.076 (3)	0.039 (2)	0.081 (3)	0.0120 (18)	0.005 (2)	0.0083 (18)
C39	0.053 (2)	0.0399 (18)	0.0426 (17)	0.0055 (15)	−0.0090 (15)	−0.0030 (14)
C40	0.0395 (16)	0.0356 (16)	0.0291 (14)	0.0040 (13)	−0.0049 (12)	−0.0017 (12)

Geometric parameters (Å, º)

O1—C14	1.360 (3)	O5—C34	1.356 (3)
O1—C15	1.449 (3)	O5—C35	1.448 (3)
O2—C15	1.397 (3)	O6—C35	1.397 (3)
O2—H2	0.89 (4)	O6—H6A	0.86 (4)
O3—C19	1.208 (4)	O7—C39	1.209 (4)
O4—C10	1.236 (4)	O8—C30	1.232 (3)
F1—C1	1.313 (4)	F4—C21	1.335 (4)
F2—C1	1.340 (5)	F5—C21	1.319 (4)
F3—C1	1.316 (4)	F6—C21	1.297 (4)
C1—C2	1.489 (5)	C21—C22	1.485 (4)
C2—C3	1.395 (5)	C22—C23	1.390 (4)
C2—C7	1.399 (4)	C22—C27	1.403 (4)
C3—C4	1.369 (5)	C23—C24	1.370 (5)
C3—H3	0.9300	C23—H23	0.9300
C4—C5	1.372 (5)	C24—C25	1.375 (5)
C4—H4	0.9300	C24—H24	0.9300
C5—C6	1.374 (4)	C25—C26	1.373 (4)
C5—H5	0.9300	C25—H25	0.9300
C6—C7	1.389 (4)	C26—C27	1.395 (4)
C6—H6	0.9300	C26—H26	0.9300
C7—C8	1.533 (4)	C27—C28	1.534 (4)
C8—C9	1.505 (4)	C28—C29	1.513 (4)
C8—C20	1.543 (4)	C28—C40	1.533 (4)
C8—H8	0.9800	C28—H28	0.9800
C9—C14	1.340 (4)	C29—C34	1.342 (4)
C9—C10	1.457 (4)	C29—C30	1.452 (4)
C10—C11	1.499 (4)	C30—C31	1.501 (4)
C11—C12	1.504 (5)	C31—C32	1.511 (5)
C11—H11A	0.9700	C31—H31A	0.9700
C11—H11B	0.9700	C31—H31B	0.9700

C12—C13	1.502 (4)	C32—C33	1.511 (4)
C12—H12A	0.9700	C32—H32A	0.9700
C12—H12B	0.9700	C32—H32B	0.9700
C13—C14	1.495 (4)	C33—C34	1.493 (4)
C13—H13A	0.9700	C33—H33A	0.9700
C13—H13B	0.9700	C33—H33B	0.9700
C15—C16	1.511 (4)	C35—C36	1.507 (4)
C15—C20	1.537 (4)	C35—C40	1.531 (4)
C16—C17	1.511 (4)	C36—C37	1.514 (5)
C16—H16A	0.9700	C36—H36A	0.9700
C16—H16B	0.9700	C36—H36B	0.9700
C17—C18	1.525 (5)	C37—C38	1.522 (5)
C17—H17A	0.9700	C37—H37A	0.9700
C17—H17B	0.9700	C37—H37B	0.9700
C18—C19	1.501 (4)	C38—C39	1.497 (5)
C18—H18A	0.9700	C38—H38A	0.9700
C18—H18B	0.9700	C38—H38B	0.9700
C19—C20	1.521 (4)	C39—C40	1.526 (4)
C20—H20	0.9800	C40—H40	0.9800

C14—O1—C15	118.1 (2)	C34—O5—C35	117.9 (2)
C15—O2—H2	111 (2)	C35—O6—H6A	113 (2)
F1—C1—F3	106.8 (3)	F6—C21—F5	106.4 (3)
F1—C1—F2	103.2 (4)	F6—C21—F4	105.5 (3)
F3—C1—F2	104.1 (3)	F5—C21—F4	102.5 (3)
F1—C1—C2	115.3 (3)	F6—C21—C22	114.6 (3)
F3—C1—C2	113.7 (4)	F5—C21—C22	114.6 (3)
F2—C1—C2	112.6 (3)	F4—C21—C22	112.1 (3)
C3—C2—C7	120.4 (3)	C23—C22—C27	120.6 (3)
C3—C2—C1	117.2 (3)	C23—C22—C21	116.4 (3)
C7—C2—C1	122.4 (3)	C27—C22—C21	123.0 (3)
C4—C3—C2	120.8 (3)	C24—C23—C22	120.7 (3)
C4—C3—H3	119.6	C24—C23—H23	119.6
C2—C3—H3	119.6	C22—C23—H23	119.6
C3—C4—C5	119.4 (3)	C23—C24—C25	119.5 (3)
C3—C4—H4	120.3	C23—C24—H24	120.2
C5—C4—H4	120.3	C25—C24—H24	120.2
C4—C5—C6	120.2 (4)	C26—C25—C24	120.3 (3)
C4—C5—H5	119.9	C26—C25—H25	119.9
C6—C5—H5	119.9	C24—C25—H25	119.9
C5—C6—C7	122.2 (3)	C25—C26—C27	121.9 (3)
C5—C6—H6	118.9	C25—C26—H26	119.0
C7—C6—H6	118.9	C27—C26—H26	119.0
C6—C7—C2	116.9 (3)	C26—C27—C22	116.9 (3)
C6—C7—C8	120.1 (3)	C26—C27—C28	120.2 (2)
C2—C7—C8	123.0 (3)	C22—C27—C28	122.9 (2)
C9—C8—C7	114.0 (2)	C29—C28—C40	109.5 (2)
C9—C8—C20	109.2 (2)	C29—C28—C27	113.3 (2)

C7—C8—C20	114.2 (2)	C40—C28—C27	114.6 (2)
C9—C8—H8	106.3	C29—C28—H28	106.3
C7—C8—H8	106.3	C40—C28—H28	106.3
C20—C8—H8	106.3	C27—C28—H28	106.3
C14—C9—C10	118.2 (3)	C34—C29—C30	118.6 (2)
C14—C9—C8	123.1 (3)	C34—C29—C28	122.7 (2)
C10—C9—C8	118.5 (2)	C30—C29—C28	118.6 (2)
O4—C10—C9	119.8 (3)	O8—C30—C29	120.0 (3)
O4—C10—C11	121.3 (3)	O8—C30—C31	121.4 (3)
C9—C10—C11	118.9 (3)	C29—C30—C31	118.7 (3)
C10—C11—C12	112.9 (3)	C30—C31—C32	111.7 (3)
C10—C11—H11A	109.0	C30—C31—H31A	109.3
C12—C11—H11A	109.0	C32—C31—H31A	109.3
C10—C11—H11B	109.0	C30—C31—H31B	109.3
C12—C11—H11B	109.0	C32—C31—H31B	109.3
H11A—C11—H11B	107.8	H31A—C31—H31B	107.9
C13—C12—C11	111.0 (3)	C31—C32—C33	110.2 (3)
C13—C12—H12A	109.4	C31—C32—H32A	109.6
C11—C12—H12A	109.4	C33—C32—H32A	109.6
C13—C12—H12B	109.4	C31—C32—H32B	109.6
C11—C12—H12B	109.4	C33—C32—H32B	109.6
H12A—C12—H12B	108.0	H32A—C32—H32B	108.1
C14—C13—C12	112.1 (3)	C34—C33—C32	111.7 (2)
C14—C13—H13A	109.2	C34—C33—H33A	109.3
C12—C13—H13A	109.2	C32—C33—H33A	109.3
C14—C13—H13B	109.2	C34—C33—H33B	109.3
C12—C13—H13B	109.2	C32—C33—H33B	109.3
H13A—C13—H13B	107.9	H33A—C33—H33B	107.9
C9—C14—O1	124.2 (3)	C29—C34—O5	124.1 (2)
C9—C14—C13	125.6 (3)	C29—C34—C33	125.3 (3)
O1—C14—C13	110.2 (2)	O5—C34—C33	110.7 (2)
O2—C15—O1	109.4 (2)	O6—C35—O5	109.8 (2)
O2—C15—C16	109.2 (2)	O6—C35—C36	111.1 (2)
O1—C15—C16	105.1 (2)	O5—C35—C36	104.7 (2)
O2—C15—C20	110.2 (2)	O6—C35—C40	107.9 (2)
O1—C15—C20	109.8 (2)	O5—C35—C40	109.9 (2)
C16—C15—C20	113.1 (2)	C36—C35—C40	113.4 (2)
C17—C16—C15	113.4 (2)	C35—C36—C37	112.5 (3)
C17—C16—H16A	108.9	C35—C36—H36A	109.1
C15—C16—H16A	108.9	C37—C36—H36A	109.1
C17—C16—H16B	108.9	C35—C36—H36B	109.1
C15—C16—H16B	108.9	C37—C36—H36B	109.1
H16A—C16—H16B	107.7	H36A—C36—H36B	107.8
C16—C17—C18	110.5 (3)	C36—C37—C38	110.3 (3)
C16—C17—H17A	109.5	C36—C37—H37A	109.6
C18—C17—H17A	109.5	C38—C37—H37A	109.6
C16—C17—H17B	109.5	C36—C37—H37B	109.6
C18—C17—H17B	109.5	C38—C37—H37B	109.6

H17A—C17—H17B	108.1	H37A—C37—H37B	108.1
C19—C18—C17	109.2 (3)	C39—C38—C37	111.2 (3)
C19—C18—H18A	109.8	C39—C38—H38A	109.4
C17—C18—H18A	109.8	C37—C38—H38A	109.4
C19—C18—H18B	109.8	C39—C38—H38B	109.4
C17—C18—H18B	109.8	C37—C38—H38B	109.4
H18A—C18—H18B	108.3	H38A—C38—H38B	108.0
O3—C19—C18	122.5 (3)	O7—C39—C38	122.3 (3)
O3—C19—C20	122.2 (3)	O7—C39—C40	122.2 (3)
C18—C19—C20	115.3 (3)	C38—C39—C40	115.4 (3)
C19—C20—C15	110.1 (2)	C39—C40—C35	110.9 (2)
C19—C20—C8	111.7 (2)	C39—C40—C28	111.4 (2)
C15—C20—C8	112.8 (2)	C35—C40—C28	112.7 (2)
C19—C20—H20	107.3	C39—C40—H40	107.2
C15—C20—H20	107.3	C35—C40—H40	107.2
C8—C20—H20	107.3	C28—C40—H40	107.2

F1—C1—C2—C3	−127.2 (4)	F6—C21—C22—C23	10.0 (5)
F3—C1—C2—C3	−3.5 (5)	F5—C21—C22—C23	133.4 (3)
F2—C1—C2—C3	114.6 (4)	F4—C21—C22—C23	−110.3 (3)
F1—C1—C2—C7	53.7 (5)	F6—C21—C22—C27	−171.5 (3)
F3—C1—C2—C7	177.5 (3)	F5—C21—C22—C27	−48.1 (4)
F2—C1—C2—C7	−64.4 (4)	F4—C21—C22—C27	68.2 (4)
C7—C2—C3—C4	0.1 (5)	C27—C22—C23—C24	−0.6 (5)
C1—C2—C3—C4	−179.0 (3)	C21—C22—C23—C24	177.9 (3)
C2—C3—C4—C5	1.7 (5)	C22—C23—C24—C25	0.1 (5)
C3—C4—C5—C6	−1.5 (5)	C23—C24—C25—C26	0.4 (5)
C4—C5—C6—C7	−0.6 (5)	C24—C25—C26—C27	−0.3 (5)
C5—C6—C7—C2	2.4 (4)	C25—C26—C27—C22	−0.2 (4)
C5—C6—C7—C8	−177.8 (3)	C25—C26—C27—C28	−179.1 (3)
C3—C2—C7—C6	−2.1 (4)	C23—C22—C27—C26	0.7 (4)
C1—C2—C7—C6	176.9 (3)	C21—C22—C27—C26	−177.8 (3)
C3—C2—C7—C8	178.1 (3)	C23—C22—C27—C28	179.5 (3)
C1—C2—C7—C8	−2.9 (5)	C21—C22—C27—C28	1.1 (4)
C6—C7—C8—C9	−27.4 (4)	C26—C27—C28—C29	26.8 (4)
C2—C7—C8—C9	152.4 (3)	C22—C27—C28—C29	−152.0 (3)
C6—C7—C8—C20	99.1 (3)	C26—C27—C28—C40	−99.8 (3)
C2—C7—C8—C20	−81.1 (3)	C22—C27—C28—C40	81.3 (3)
C7—C8—C9—C14	118.2 (3)	C40—C28—C29—C34	9.8 (4)
C20—C8—C9—C14	−10.9 (4)	C27—C28—C29—C34	−119.5 (3)
C7—C8—C9—C10	−66.8 (3)	C40—C28—C29—C30	−166.5 (2)
C20—C8—C9—C10	164.1 (2)	C27—C28—C29—C30	64.2 (3)
C14—C9—C10—O4	174.8 (3)	C34—C29—C30—O8	−176.2 (3)
C8—C9—C10—O4	−0.4 (4)	C28—C29—C30—O8	0.2 (4)
C14—C9—C10—C11	−5.8 (4)	C34—C29—C30—C31	4.6 (4)
C8—C9—C10—C11	179.0 (3)	C28—C29—C30—C31	−179.0 (3)
O4—C10—C11—C12	−147.7 (3)	O8—C30—C31—C32	146.2 (3)
C9—C10—C11—C12	32.9 (4)	C29—C30—C31—C32	−34.6 (4)

C10—C11—C12—C13	−52.5 (4)	C30—C31—C32—C33	55.5 (4)
C11—C12—C13—C14	45.6 (4)	C31—C32—C33—C34	−47.2 (4)
C10—C9—C14—O1	−179.8 (3)	C30—C29—C34—O5	−177.9 (2)
C8—C9—C14—O1	−4.8 (4)	C28—C29—C34—O5	5.8 (4)
C10—C9—C14—C13	−0.7 (4)	C30—C29—C34—C33	3.8 (4)
C8—C9—C14—C13	174.4 (3)	C28—C29—C34—C33	−172.5 (3)
C15—O1—C14—C9	−11.2 (4)	C35—O5—C34—C29	11.3 (4)
C15—O1—C14—C13	169.5 (2)	C35—O5—C34—C33	−170.3 (2)
C12—C13—C14—C9	−20.2 (4)	C32—C33—C34—C29	18.5 (4)
C12—C13—C14—O1	159.1 (3)	C32—C33—C34—O5	−159.9 (3)
C14—O1—C15—O2	−80.5 (3)	C34—O5—C35—O6	77.2 (3)
C14—O1—C15—C16	162.4 (2)	C34—O5—C35—C36	−163.4 (2)
C14—O1—C15—C20	40.5 (3)	C34—O5—C35—C40	−41.4 (3)
O2—C15—C16—C17	174.2 (2)	O6—C35—C36—C37	−175.2 (3)
O1—C15—C16—C17	−68.5 (3)	O5—C35—C36—C37	66.4 (3)
C20—C15—C16—C17	51.2 (3)	C40—C35—C36—C37	−53.5 (3)
C15—C16—C17—C18	−55.8 (4)	C35—C36—C37—C38	56.6 (4)
C16—C17—C18—C19	56.8 (4)	C36—C37—C38—C39	−55.3 (4)
C17—C18—C19—O3	120.7 (4)	C37—C38—C39—O7	−127.0 (3)
C17—C18—C19—C20	−56.9 (4)	C37—C38—C39—C40	52.5 (4)
O3—C19—C20—C15	−126.0 (3)	O7—C39—C40—C35	131.7 (3)
C18—C19—C20—C15	51.6 (3)	C38—C39—C40—C35	−47.7 (3)
O3—C19—C20—C8	0.2 (4)	O7—C39—C40—C28	5.3 (4)
C18—C19—C20—C8	177.8 (3)	C38—C39—C40—C28	−174.2 (3)
O2—C15—C20—C19	−169.5 (2)	O6—C35—C40—C39	170.8 (2)
O1—C15—C20—C19	70.0 (3)	O5—C35—C40—C39	−69.5 (3)
C16—C15—C20—C19	−47.0 (3)	C36—C35—C40—C39	47.3 (3)
O2—C15—C20—C8	65.0 (3)	O6—C35—C40—C28	−63.5 (3)
O1—C15—C20—C8	−55.6 (3)	O5—C35—C40—C28	56.2 (3)
C16—C15—C20—C8	−172.6 (2)	C36—C35—C40—C28	173.0 (2)
C9—C8—C20—C19	−84.5 (3)	C29—C28—C40—C39	85.6 (3)
C7—C8—C20—C19	146.6 (2)	C27—C28—C40—C39	−145.8 (2)
C9—C8—C20—C15	40.2 (3)	C29—C28—C40—C35	−39.8 (3)
C7—C8—C20—C15	−88.7 (3)	C27—C28—C40—C35	88.8 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2···O8^{i}	0.89 (4)	1.82 (4)	2.704 (3)	172 (3)
C11—H11*A*···F4^{i}	0.97	2.51	3.307 (5)	140
C16—H16*B*···O2^{ii}	0.97	2.52	3.403 (4)	152
C20—H20···F1	0.98	2.40	2.960 (4)	116
O6—H6*A*···O4	0.86 (4)	1.83 (4)	2.684 (3)	171 (3)
C36—H36*B*···O6^{iii}	0.97	2.59	3.473 (4)	152
C40—H40···F5	0.98	2.35	2.901 (4)	115

Symmetry codes: (i) *x*−1, *y*, *z*; (ii) −*x*, −*y*+2, −*z*+1; (iii) −*x*+1, −*y*+1, −*z*+2.